On The Electronic Properties of Photoacids In The Gas Phase.

Electric Dipole Moments of CIS- and TRANS-2-Naphthol

ADAM FLEISHER, PHILIP MORGAN, DAVID PRATT, University of Pittsburgh — The permanent electric dipole moments ($\mu$) of two conformers of 2-naphthol (2HN) in their ground and electronically excited states have been experimentally determined by Stark-effect measurements in a molecular beam. Upon UV excitation, little change in the magnitudes of $\mu$ is observed, but the orientation of the dipole moment within each conformer shifts significantly, indicating photon-induced rearrangements in electronic distributions. cis-2HN has $\Delta \mu = +0.17$ D and $\Delta \theta_a = -28^\circ$ and trans-2HN has $\Delta \mu = +0.05$ D and $\Delta \theta_a = +28^\circ$ (trans-2HN). The $\Delta \theta_a$ values for the two conformers differ in sign. The small changes in the magnitudes of the dipole moments suggest that the isolated molecules do not undergo large charge separations upon excitation. Our study, void of solvent perturbations, is of importance to the larger community currently describing aromatic biomolecule and “super” photoacid behavior via theoretical modeling and condensed phase solvatochromism.

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